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# Scattering of light on the surfaces of photonic crystals

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## Abstract

We present a new method to calculate the scattering of light at the surface of a photonic crystal. The problem is solved in terms of virtual surface-current distributions and the calculation takes full advantage of the existing infinite-space plane-wave expansion method for obtaining the photonic band structure. Working with surface currents makes the calculations less time-consuming by means of reduction of the dimensionality in the problem. The method is tested and illustrated for semi-infinite two-dimensional photonic crystals of small and large dielectric contrast. © 2002 Elsevier Science B.V. All rights reserved.

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The multiple scattering of waves in complex media is one of the intriguing problems in physics. A situation of considerable importance to which this problem is relevant, concerns the propagation of light in photonic crystals. These are materials with a spatially periodic index of refraction. Their dispersion relation  $\omega(\mathbf{k})$  is described by the photonic band structure, which consists of different bands, showing gaps between them at the boundary of the Brillouin zone. Fascinating fundamental effects (e.g. localisation of light, control of spontaneous emission [1–4]) as well as prospective technological applications (e.g. low-threshold lasers, single-mode lossless waveguides [2,5,6]) explain the enormous interest in photonic crystals and photonic band structures [7–10].

While most of the theoretical effort in this field has been devoted to calculating band structures and densities of states for ideal infinite crystals [7,11–15], the notoriously complicated problem of accounting for scattering of light on the crystal's surfaces has received relatively little attention. Yet, any experiment or future device necessarily involves such scattering and the finiteness of the crystal. Methods that have been developed, include the generalised field-propagator method [16] and the transfer-matrix method [17,18]. The former formulates the scattering problem in terms of three-dimensional vector integral equations, whose numerical solution is a time-consuming process. The latter assumes that the crystal can be built up from thin infinite layers and has as disadvantage that it is restricted to slab structures.

In this paper, we present a rigorous alternative method, which is generally applicable to two- and three-dimensional crystals of arbitrary shape and to incident monochromatic fields of arbitrary

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spatial form. Independent of size and shape of the crystal, the method uses as input the infinite-space photonic band structure. The crux of our method is the representation of the electromagnetic fields inside a medium in terms of a single surface-current distribution just inside the boundary surface of the medium. The fact that one surface current suffices is a non-trivial extension of the classical representation theorem, which states that in an arbitrary linear medium monochromatic electromagnetic fields of frequency  $\omega$  may be written in terms of two surface- and two volume-current distributions [19,20]:

$$\mathbf{H}(\mathbf{r}) = \int_V \left[ -i\omega\mu\mathbf{M}_v G - \mathbf{J}_v \times \nabla' G + \frac{\rho_v}{\varepsilon} \nabla' G \right] d\mathbf{r}' + \int_S \left[ -i\omega\mu\mathbf{J}_s G - \mathbf{M}_s \times \nabla' G + \frac{\rho_s}{\varepsilon} \nabla' G \right] d\mathbf{r}'. \quad (1)$$

Here, the first (second) integral extends over the volume  $V$  (boundary  $S$ ) of the medium. Furthermore,  $G$  stands for  $G(\mathbf{r}, \mathbf{r}')$  and denotes an arbitrary scalar Green's function satisfying  $(\nabla^2 + (\omega/c)^2)G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$ . All other functions in the integrands are to be taken at  $\mathbf{r}'$ ;  $\nabla'$  stands for differentiation with respect to  $\mathbf{r}'$ .

In Eq. (1),  $\mu$  and  $\varepsilon$  are the (position dependent) magnetic permeability and dielectric permittivity in the medium, while the sources of the fields (the “equivalent currents”) have the explicit form:  $\mathbf{M}_v = i\omega(\mu_0 - \mu)\mathbf{H}$ ,  $\mathbf{J}_v = i\omega(\varepsilon_0 - \varepsilon)\mathbf{E}$ ,  $\mathbf{J}_s = \mathbf{n} \times \mathbf{E}_s$  and  $\mathbf{M}_s = \mathbf{n} \times \mathbf{H}_s$ . Here,  $\mathbf{n}$  is the normal to  $S$  and  $\mu_0$  and  $\varepsilon_0$  are the magnetic permeability and electric permittivity of the vacuum, respectively. Finally, using the continuity equation, the equivalent charge densities may be expressed as  $\rho_{s,v} = i\omega\nabla \cdot \mathbf{J}_{s,v}$ .

Clearly, if we consider the fields in a vacuum region, only the surface currents survive. In fact, however, for any homogeneous medium with index of refraction  $n \equiv \sqrt{\mu\varepsilon/\mu_0\varepsilon_0}$ , we may eliminate the volume currents ( $\mathbf{M}_v$  and  $\mathbf{J}_v$ ) from the representation by using inside the medium the free-space Green's function with  $\omega/c$  replaced by  $n\omega/c$ . Thus, the scattering of light on the interface between vacuum and a homogeneous medium, may be rewritten in terms of four surface-current dis-

tributions, two on the vacuum side and two on the medium side of the interface. If the medium is a perfect conductor, the situation simplifies even more, as then  $\mathbf{n} \times \mathbf{E}_s = 0$ , leaving us with only one surface current ( $\mathbf{M}_s$ ). In this case,  $\mathbf{M}_s$  is in fact a real current and expressing the fields in terms of it and applying the Maxwell boundary conditions is a familiar method to solve for  $\mathbf{M}_s$  and thereby solve the scattering problem on perfect conductors [21].

Even though photonic crystals are by their very nature not homogeneous and often not conducting, a similar strategy of field representation and solution can be applied to these materials. The volume currents can be eliminated by using the appropriate Green's tensor for the electromagnetic field inside the periodic medium, which may be expressed in terms of the standard Bloch modes (see below). This leaves us with a field representation in terms of two surface currents on either side of  $S$ . It may be shown, however, that the term  $-\mathbf{M}_s \times \nabla' G + (\rho_s/\varepsilon)\nabla' G$  in the surface integral can always be rewritten in terms of  $-i\omega\mu\tilde{\mathbf{J}}'_s G$  for a suitable choice of the current  $\tilde{\mathbf{J}}'_s$ . This “equivalence of current- and dipole-layer representations” has a well-known electrostatic analogue [22]. The detailed technical proof for the Maxwell fields follows similar lines and will be given elsewhere [24].

Thus we arrive at a field representation with just one surface current on each side of the crystal's surface  $S$  (see Fig. 1). Explicitly, we may write the magnetic field on the vacuum side

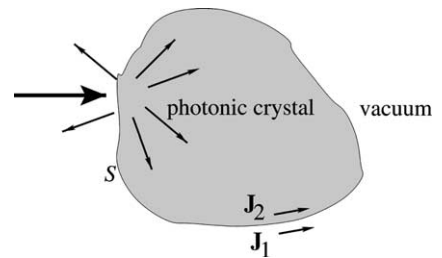


Fig. 1. Scattering of light by a photonic crystal. The electromagnetic fields outside the crystal are generated by the virtual current  $\mathbf{J}_1$  on the outside of the boundary surface  $S$ . The fields inside the crystal are generated by  $\mathbf{J}_2$ .

$$\mathbf{H}_1(\mathbf{r}) = \mathbf{H}_{\text{inc}}(\mathbf{r}) + \int_S \vec{\Gamma}(\mathbf{r}, \mathbf{r}'_S, \omega) \mathbf{J}_1(\mathbf{r}'_S) d\mathbf{r}'_S. \quad (2)$$

Here,  $\mathbf{H}_{\text{inc}}(\mathbf{r})$  is the incident external field, which we keep explicitly, i.e., we do not express it in terms of surface currents. Furthermore,  $\vec{\Gamma}$  is the dyadic Green's tensor for electromagnetic waves in vacuum, which depends on the dimensionality of the problem and satisfies Sommerfeld's radiation condition (see [23, pp. 247–248]), as is appropriate to describe outgoing waves. Similarly, on the crystal side of the interface  $S$ , the magnetic field is expressed as

$$\mathbf{H}_2(\mathbf{r}) = \int_S \vec{\mathcal{G}}(\mathbf{r}, \mathbf{r}'_S, \omega) \mathbf{J}_2(\mathbf{r}'_S) d\mathbf{r}'_S, \quad (3)$$

where  $\vec{\mathcal{G}}$  is the dyadic Green's tensor for the infinite photonic crystal, which reads (as in [25], using  $\nabla \cdot \mathbf{H} = 0$ )

$$\vec{\mathcal{G}}(\mathbf{r}, \mathbf{r}'_S, \omega) = \sum_n \int_{\text{1BZ}} \frac{\tilde{\mathbf{h}}_n(\mathbf{r}; \mathbf{k}) \otimes \tilde{\mathbf{h}}_n^*(\mathbf{r}'_S; \mathbf{k})}{((\omega_n(\mathbf{k}))^2 - \omega^2 + \gamma^2 + 2i\gamma\omega)/c^2} d\mathbf{k}. \quad (4)$$

Here  $\tilde{\mathbf{h}}_n(\mathbf{r}; \mathbf{k})$  are the normalised Bloch modes

$$\tilde{\mathbf{h}}_n(\mathbf{r}; \mathbf{k}) \equiv \sum_m \sum_{\lambda=1}^2 \tilde{h}_{m\lambda}^{(n)}(\mathbf{k}) \hat{\mathbf{u}}_m^\lambda e^{-i\mathbf{k}_m \cdot \mathbf{r}}, \quad (5)$$

which for a non-magnetic medium ( $\mu = \mu_0$ ) are defined uniquely by the equation

$$\nabla \times \left( \frac{\varepsilon_0}{\varepsilon(\mathbf{r})} \nabla \times \tilde{\mathbf{h}}_n(\mathbf{r}; \mathbf{k}) \right) = \frac{\omega_n^2}{c^2} \tilde{\mathbf{h}}_n(\mathbf{r}; \mathbf{k}) \quad (6)$$

and the condition that the fields are bounded at  $|\mathbf{r}| \rightarrow \infty$ . The index  $n$  is used for labelling the eigenfrequencies  $\omega_n$  and the eigenvectors  $\tilde{h}_{m\lambda}^{(n)}(\mathbf{k})$ . These Bloch modes are the eigenvectors, which are calculated in the standard plane-wave expansion method, that is used to obtain the photonic band structure [7,11]. By  $\hat{\mathbf{u}}_m^\lambda$ ,  $\lambda = 1, 2, 3$ , we denote an orthonormal basis for Euclidian space, for each index  $m$  which labels a reciprocal-lattice vector  $\mathbf{g}_m$ . By the vector  $\mathbf{k}_m$  we denote  $\mathbf{k} + \mathbf{g}_m$ . The small absorption parameter  $\gamma$  in  $\vec{\mathcal{G}}$  has been introduced to handle its singularity along the dispersion curves in  $\mathbf{k}$ -space.

The field representations Eqs. (2) and (3) can be used now to solve the scattering of light on the

photonic crystal. To this end, the two surface currents  $\mathbf{J}_1$  and  $\mathbf{J}_2$  are understood to be unknown (virtual) currents, which can be solved by imposing the continuity of the tangential components of the resulting magnetic and electric fields across  $S$  (the electric fields simply follow from  $\mathbf{E} = -i\nabla \times (\mathbf{B}/\mu)/(\omega\varepsilon)$ ). This leads to an inhomogeneous set of linear equations for  $\mathbf{J}_1$  and  $\mathbf{J}_2$ , in which the incident field is responsible for the inhomogeneity (the source term). Solution of these equations (in practice most easily performed by discretising the current distributions) suffices to obtain the fields everywhere. We note that for a  $d$ -dimensional photonic crystal, the equations for the surface currents have a dimensionality of only  $d-1$ , which is an important computational advantage of our method.

Thus, in practice our method involves (i) the construction of the Green's tensor of the photonic crystal using standard band-structure calculations, (ii) the solution of a set of linear equations for the discretised surface-current distributions and (iii) the calculation of the fields of interest using the solution obtained for the currents.

Before we turn to applications of our method, we wish to point out that it applies to more general situations than considered above. For example, we may equally well use it to describe the scattering of light produced by a source inside the photonic crystal, as would be appropriate for radiative emission processes in light-emitting diodes and experiments on the control of spontaneous emission. To this end, we simply remove the incident field on the vacuum side and add a source term on the crystal side representing the current associated with the oscillating dipole that produces the radiation. Yet another situation that may be described using our field representation, is one in which real volume currents,  $\mathbf{J}_v$ , produced by a beam of moving particles, occur. To consider such a situation, which applies to, e.g., electron energy loss experiments, one simply adds terms sourced by the explicit volume currents to the fields inside and (or) outside the crystal. For a current outside the crystal, this yields an additional term to  $\mathbf{H}_1(\mathbf{r})$  that is given by the second term occurring in the volume integral at the right-hand side of Eq. (1), while for currents inside the crystal, the additional term

to  $\mathbf{H}_2(\mathbf{r})$  is represented by  $\nabla \times (\mathbf{J}_v/\varepsilon) \cdot \vec{\Gamma}$ . Thus, in this situation the explicit volume currents generate the inhomogeneity in the set of equations for  $\mathbf{J}_1$  and  $\mathbf{J}_2$ .

In the remainder of this paper, we illustrate our method by applying it to the problem of scattering of a light field incident on a two-dimensional (2D) non-magnetic photonic crystals filling a half space. The 2D free-space Green's tensor reads

$$\vec{\Gamma}(\mathbf{r}, \mathbf{r}', \omega) = \frac{1}{4i} (\vec{\mathcal{I}} + (c/\omega)^2 \nabla \otimes \nabla) H_0^{(2)}(\omega|\mathbf{r} - \mathbf{r}'|/c), \quad (7)$$

where  $H_0^{(2)}$  is the zeroth-order Hankel function of the second kind. The crystal under consideration has a 2D periodicity of the dielectric function  $\varepsilon(\mathbf{r})$  in the  $x$  and  $y$  directions and is infinitely extended in the  $z$  direction, see Fig. 2. The vector  $\mathbf{r}$ , that occurs in our expressions, is restricted to the  $xy$ -plane. Since, for purely 2D photonic crystals, there is no mixing between the two polarisations (TE, with the electric field perpendicular to the  $z$ -axis, and TM, with the magnetic field perpendicular to the  $z$ -axis), we have a set of only two equations for each polarisation, namely the continuity of  $\mathbf{H}_z$  and  $(\nabla \times \mathbf{H})_y$  for TE polarisation, with  $\mathbf{J}_1$  and  $\mathbf{J}_2$  being only in the  $z$  direction, and the continuity of  $\mathbf{H}_y$  and  $(\nabla \times \mathbf{H})_z$  for TM polarisation, with the surface currents  $\mathbf{J}_1$  and  $\mathbf{J}_2$  being only in the  $y$  direction.

We have used our method to reconstruct the reflected fields in the vacuum region from the surface-current distribution  $\mathbf{J}_1$ . In particular, we have calculated the distribution of the energy flow

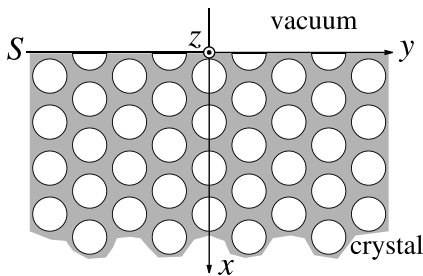


Fig. 2. Cross-section of a two-dimensional photonic crystal with the  $xy$ -plane. The boundary surface  $S$  of the crystal is defined to be the  $yz$ -plane.

over all outgoing directions  $\alpha$  (measured with respect to the surface normal), upon irradiation of the crystal by a plane wave. For this intensity distribution we use the asymptotic behaviour of  $\vec{\Gamma}$  at large distances away from the crystal surface. As a measure for the intensity we use the dimensionless quantity  $I(\alpha) \equiv D|\mathbf{H}|^2/|\mathbf{H}_{\text{in}}|^2$ , where  $D$  is the ratio of the distance at which the field is observed and the length of the crystal surface. This measure is independent of  $D$ , as for 2D systems  $|\mathbf{H}|$  is inversely proportional to  $\sqrt{D}$ .

Explicitly, we have considered the scattering of a plane-wave incident on a 2D crystal consisting of air cylinders (radius  $R = 0.48a$ ), arranged on a triangular lattice (lattice constant  $a$ ) in a dielectric background, as shown in Fig. 2. We present results for two configurations of the crystal, which differ in the value of the dielectric contrast.

Fig. 3 shows the angular distribution of the reflected intensity in the case where the dielectric background has index of refraction  $n = 1.05$ , i.e., a weakly scattering crystal. We considered a scattering surface with length  $L = 40a$ , which was discretised into 401 points. For a sufficiently accurate calculation of the Green's tensor of the crystal, we used an expansion in 283 plane waves and we performed the integration over the first

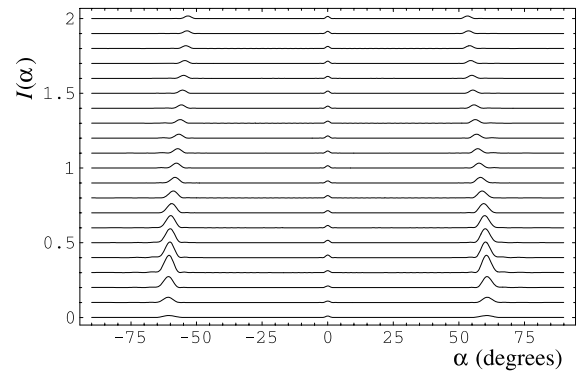


Fig. 3. Angular distribution of the intensity of the light reflected from a weakly scattering 2D photonic crystal consisting of air cylinders (radius  $R = 0.48a$ ), arranged on a triangular lattice (lattice constant  $a$ ) in a dielectric background (index of refraction  $n = 1.05$ ). The incident light consists of a TE polarised plane wave, incident normally onto the scattering surface, with frequency ranging from  $\omega = 4.071c/a$  (bottom curve, no offset) to  $\omega = 4.531c/a$  (top curve; offset 2.0), using steps of  $\Delta\omega = 0.023c/a$ .

Brillouin zone in Eq. (4) by discretising half of this BZ into 12 286 points. For the absorption rate we used  $\gamma = 0.005\omega$ . The incident plane wave was taken TE polarised and incident normally to the surface, its frequency ranging from  $\omega = 4.071c/a$  to  $\omega = 4.531c/a$ .

In Fig. 3, we observe that part of the light is reflected normal to the crystal surface. This is the specularly reflected part of the field, which for the present weak contrast is very small. In addition to this specular reflection, we observe two peaks, occurring at  $\alpha \approx \pm 60^\circ$ . These are the Bragg peaks, which follow from single scattering of the incident beam on the dielectric periodicity (first-order Born's approximation). Momentum conservation dictates that the wave vector of the outgoing beam differs from the incident one by a reciprocal-lattice vector. Because energy must be conserved as well, Bragg scattering ideally should only occur for  $\omega = \omega_0 = (4\pi/3)c/a \approx 4.189c/a$ , with scattering angles  $\alpha = \pm 60^\circ$ . This ideal situation is represented by the sixth curve from below in Fig. 3. The finite width of both peaks results from the finite length of the crystal surface  $L = 40a$ .

We observe, however, that for a range of frequencies around the resonance frequency  $\omega_0$ , the Bragg peaks survive. This is due to the finite damping rate  $\gamma$ , which may be interpreted as leading to a finite depth of the crystal, thus breaking momentum conservation in the  $x$  direction. A simple calculation, based on the conservation of momentum in the  $y$ -direction (the direction parallel to the crystal surface), shows that the angle  $\alpha$  must satisfy the relation  $\alpha = \arcsin(\frac{1}{2}\sqrt{3}\omega_0/\omega)$ . This explains accurately the shifting of the peak position in Fig. 3 from  $\alpha = \pm 61^\circ$  at  $\omega = 4.071c/a$  (bottom curve) to  $\alpha = \pm 53^\circ$  at  $\omega = 4.531c/a$  (top curve). The width of the frequency region in which the Bragg peaks can be observed agrees well with estimates based on the finite effective crystal depth imposed by  $\gamma$ . We finally note that changing the index of refraction to  $n = 1.1$  leaves the angular intensity distributions identical, except for changing the vertical scale by a factor of four, which confirms that we are in the single-scattering regime.

We have repeated these calculations for the same geometry, but with a dielectric background

of  $n = 4.0$ . For this strong-scattering case, a full band gap develops for both TE and TM polarisation, as is clearly seen in the band structure plotted in Fig. 4(a). The angular distribution of the reflected TE light for this crystal is given in Fig. 4(b) for a range of frequencies, all lying above the band gap (frequencies inside the gap give rise to complete specular reflection, as there are no Bloch modes to couple the light to). Again, we observe the specular reflection and the “Bragg” peaks, which, of course, all have a strongly increased intensity compared to the weak-scattering case. Remarkably, the range of frequencies over which the “Bragg” peaks are

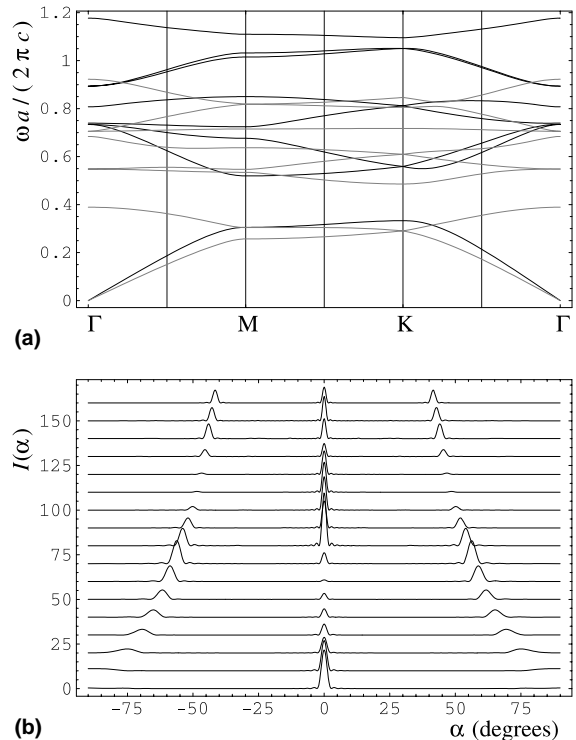


Fig. 4. (a) Band structure for the strongly scattering 2D photonic crystal with the same parameters as in Fig. 3, except that the background index of refraction is  $n = 4.0$ . The black (grey) curves correspond to the TE (TM) modes. (b) Angular distribution of the intensity of the light reflected from this 2D photonic crystal, upon irradiation by a TE plane wave of normal incidence, with frequencies ranging from  $\omega = 3.512c/a$  (bottom curve, no offset) to  $\omega = 5.464c/a$  (top curve, offset 160), using steps of  $\Delta\omega = 0.122c/a$ .

observed, has grown appreciably compared to the case of weak scattering. While we cannot give a simple theoretical estimate of this frequency range, we note that over the entire range the position of the peak is again accurately described by  $\alpha = \arcsin(\frac{1}{2}\sqrt{3}\omega_0/\omega)$ . The frequency for which the thus calculated angle becomes  $\alpha = \pm 90^\circ$ , equals  $(2\pi/\sqrt{3})c/a$ , which lies just above the stop gap in the K direction (direction of incidence) and agrees with the second curve from below in Fig. 4(b). We also note an interesting non-monotonic behaviour of the intensities of the peaks as a function of the frequency, where a redistribution of energy seems to take place between the specular and the “Bragg” peaks.

To conclude, we have presented a method to calculate the scattering of light at the surface of a photonic crystal. The scattering problem is solved in terms of virtual surface-current distributions and the calculation takes full advantage of the existing plane-wave expansion method for obtaining the photonic band structure. Working with surface currents reduces the dimensionality in the problem and thus also reduces the required computer time and memory. We have tested our method for a weakly scattering 2D photonic crystal; all results were found to agree accurately with theoretical expectations. We have also used the method for a first study on a strongly scattering crystal, where simple arguments based on Born’s approximation break down. A more extensive analysis of strongly scattering crystals, as well as the application of our method to more general situations (crystals of different shapes and incident light of non-plane-wave nature) will be the topic of further study. Finally, we have pointed out that the method may also be used to describe situations with light sources inside the photonic crystal (spontaneous emission) or with

volume currents (particle beams) acting as field sources.

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